Status of Thermal Fluid Code and Coupling with Neutronics Code in ANL

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Progress Review Meeting on Advanced Multi-Physics Simulation Capability for VHTRs

Hyatt Regency Hotel, Atlanta

June 17 – 18, 2009

Overview

- **Background**
  - VHTR M&S Challenges
  - SHARP for AFCI NEAMS
  - Current Design Practices
- **VHTR Advanced M&S Project**
  - Objectives and Approach
- **Key Achievements**
  - Thermo-fluid
  - Coupling Calculations
- **Future Work**

Challenges for VHTR Modeling and Simulation

Neutronics

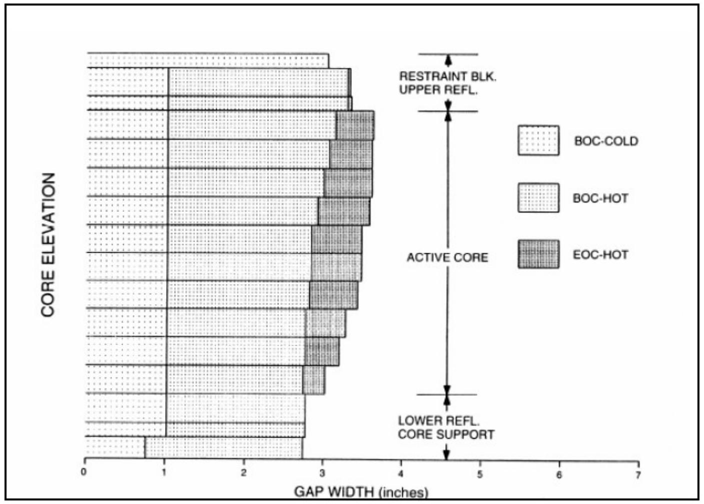
- Double heterogeneity effects due to TRISO fuel particles and compacts
- Large leakage fraction due to large migration area and annular core shape
- Strong core/reflector coupling and thermal flux peaking
- Increased importance of low lying Pu resonances and T-dependent graphite scattering kernel for deep-burn configurations

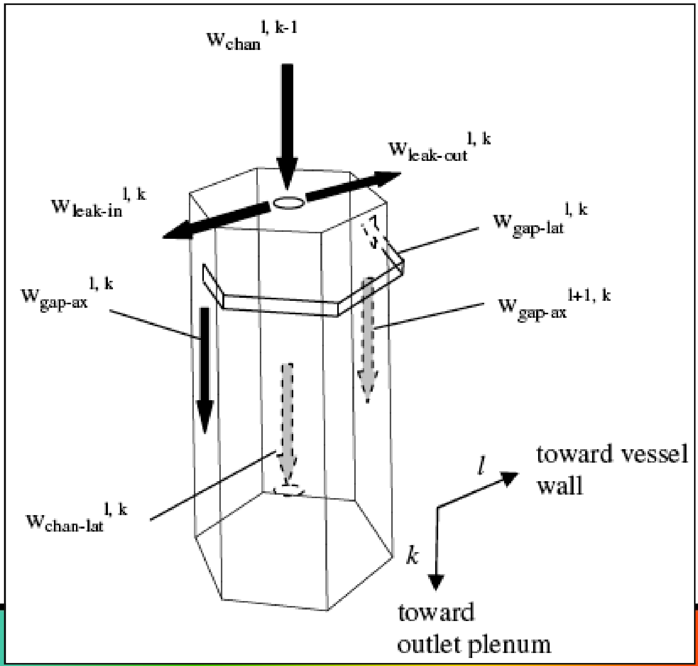
Thermo-Fluid Dynamics

- Convective heat removal by coolant flowing through fuel blocks (for various flow conditions)
- Coolant bypass of coolant channels (gap flow)
- Multidimensional conduction within blocks
- Radiative redistribution of thermal load between blocks
- Large number of coolant channels much longer than hydraulic diameter

Current Design Practices
Network Flow Solvers for Parametric Design Analysis

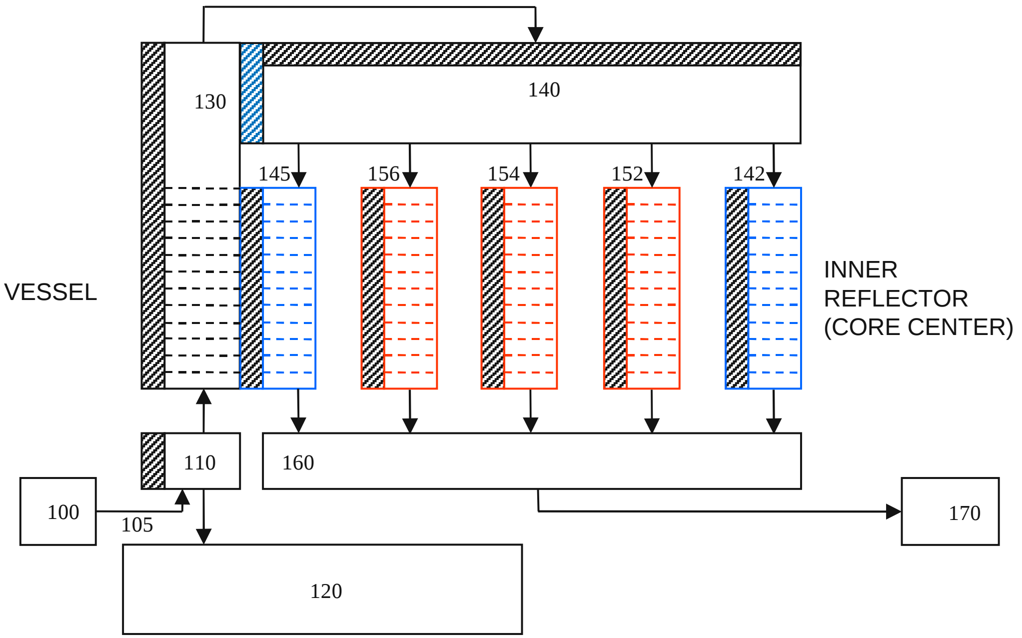
- Nodal network flow simulators are used for parametric design analysis
  - Specialized codes like GAS-NET
  - Commercial codes like Flownex
- Use same correlation database as safety codes
- Allow for direct consideration of bypass flows
  - Axial core bypass flows
  - Radial core bypass flows
  - Control rod channel leakage
  - Leakage past gap seal of core support
  - Openings in blocks at periphery
- User must define gap/leakage path dimensions and characteristics

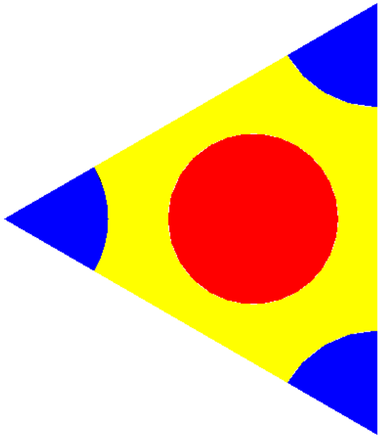


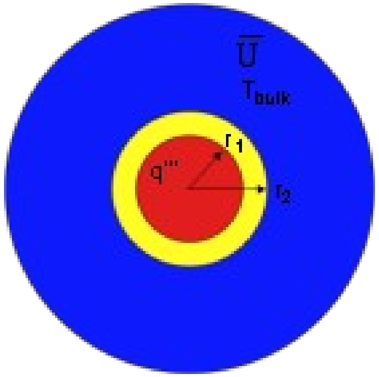


Current Design Practices
Lumped Parameter Models for Safety Analysis

- Entire VHTR core is represented as 2 - 4 characteristic channels
  - Heat and mass are conserved for the entire mass and volume of the core regions represented by each channels
  - All heat transfer is modeled as "effective" conduction
- Inner and outer reflector are each represented as a single channel
- Fuel temperatures are typically determined from 2D or 1D single channel analysis with lumped parameter representations
- Simulations based on correlations



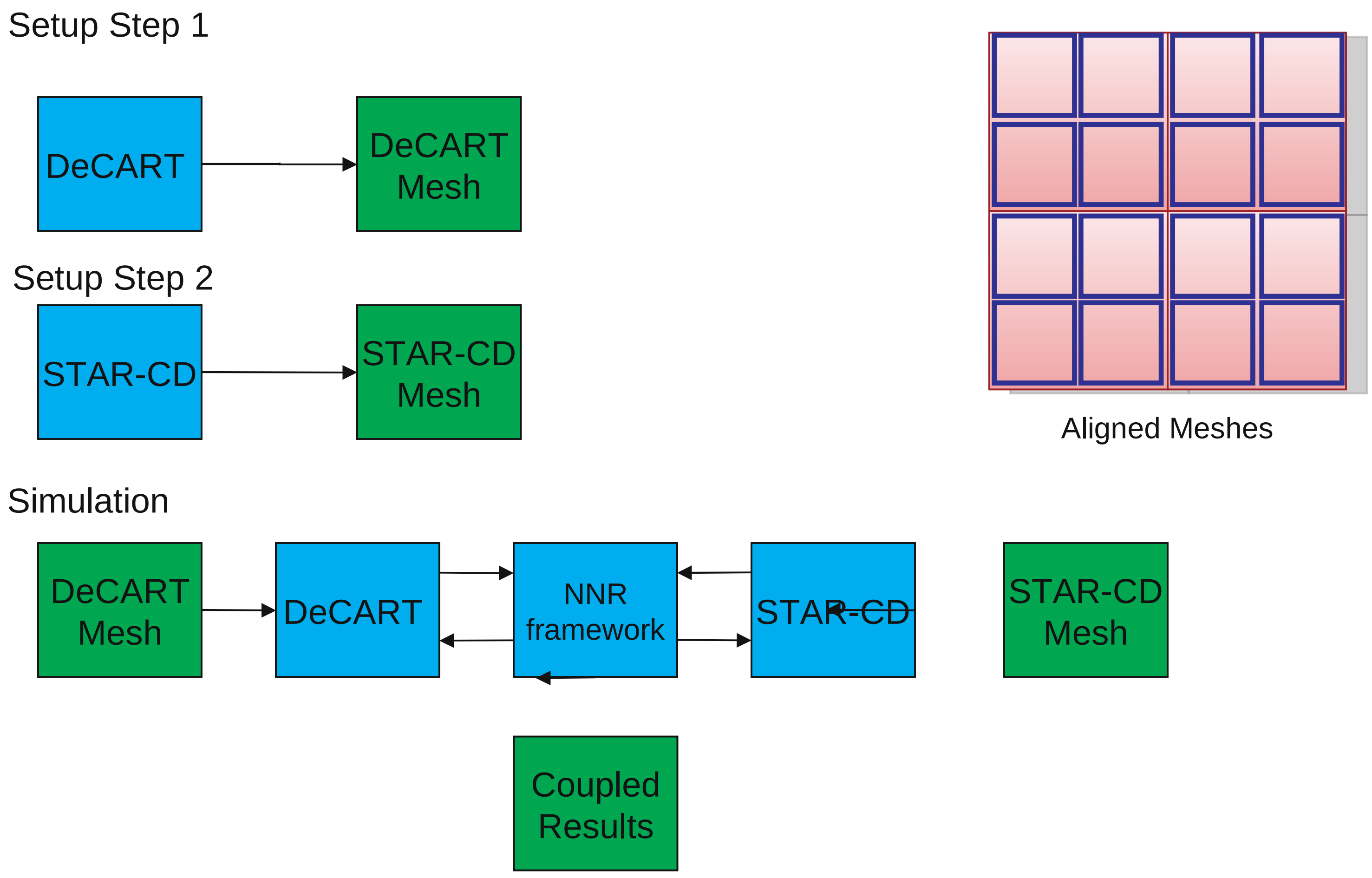




Approaches Thermofluids Analysis and Coupling

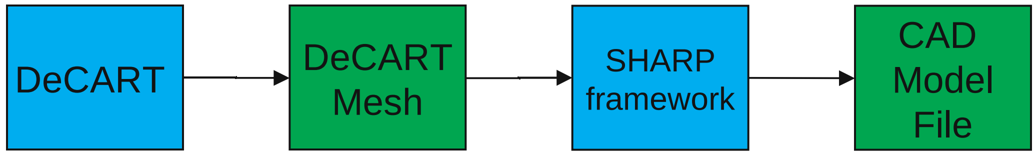
- Leverage the prior experiences of NNR high-fidelity simulation tool for LWR applications
- Incorporate the commercially-developed STAR-CD/STAR-CCM+ code suite directly into the SHARP framework to augment the capabilities provided by Nek5000 and make additional modeling improvements to satisfy the target performance
- Improve efficiency of model development
  - Enable physics-specific mesh type and resolution selection
    - *Mapping of structured and unstructured meshes*
  - Remove additional constraints on coupled model
  - Eliminate additional steps required for coupled model development
- Improve efficiency of coupled simulation
  - Enable direct communications between physics modules
  - Parallelization of data streams and data structures

NNR Model Generation and Coupling Strategy
Require that DeCART and STAR-CD meshes align



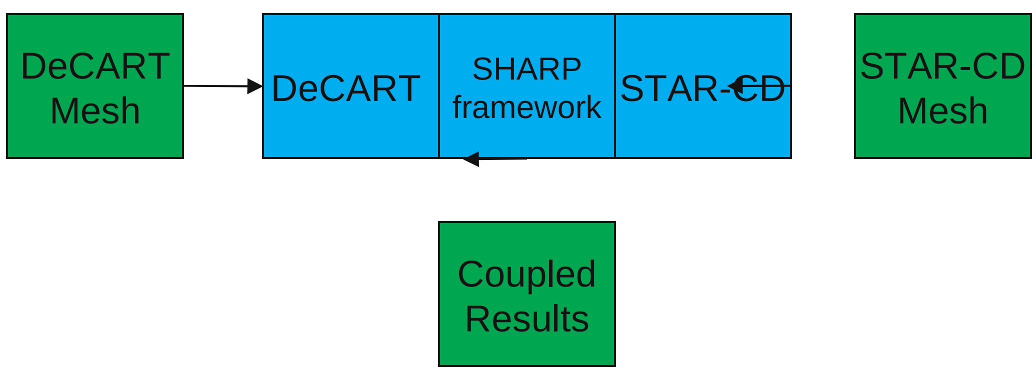
Initial Model Generation and Coupling Strategy
Require that DeCART and STAR-CD meshes align

Setup Step 1



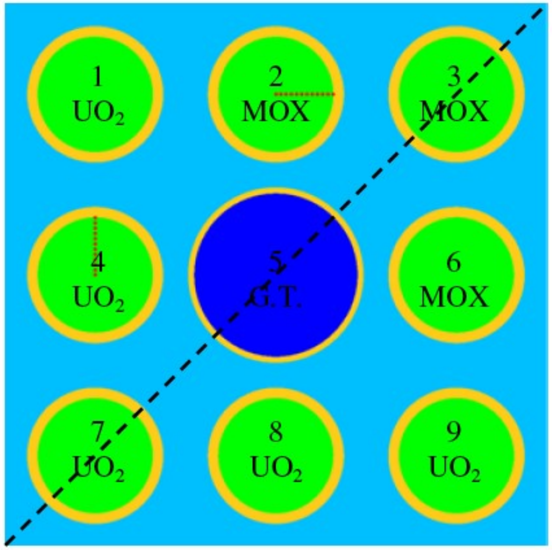
Setup Step 2

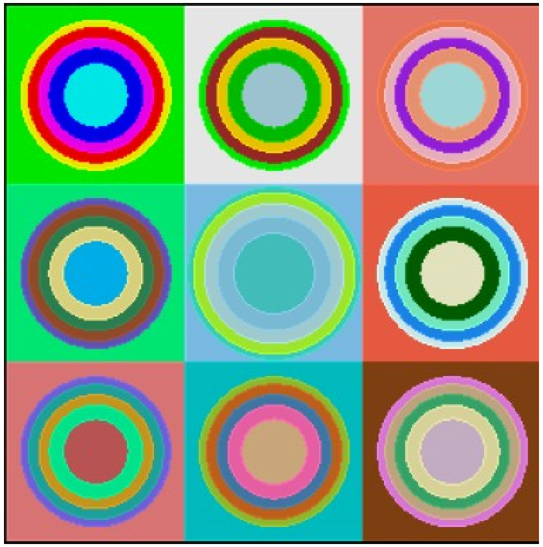
Simulation

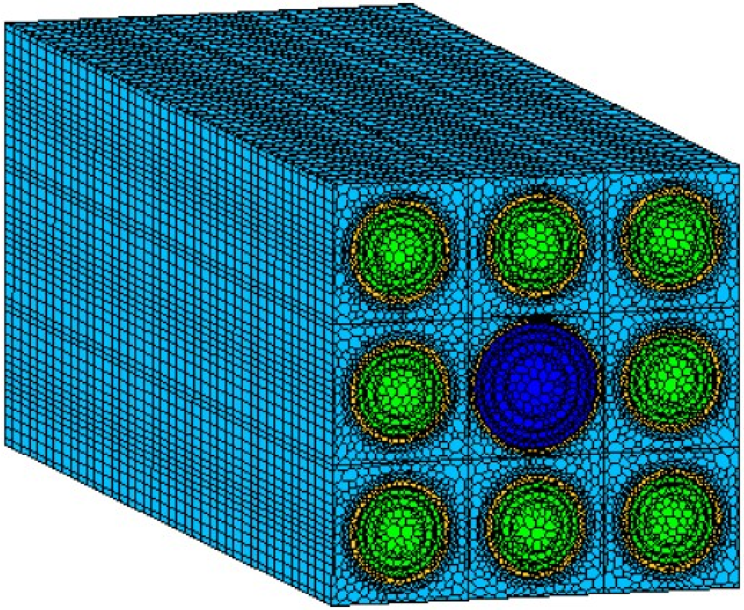


Initial Coupled Demonstration

- Use 3 x 3 LWR demonstration problem from NNR activities
- Demonstrate coupling of new versions of DeCART and STAR-CD using initial coupling strategy
  - Require that CFD meshes be aligned with DeCART meshes
  - Results in > 6 million computational cells in CFD domain

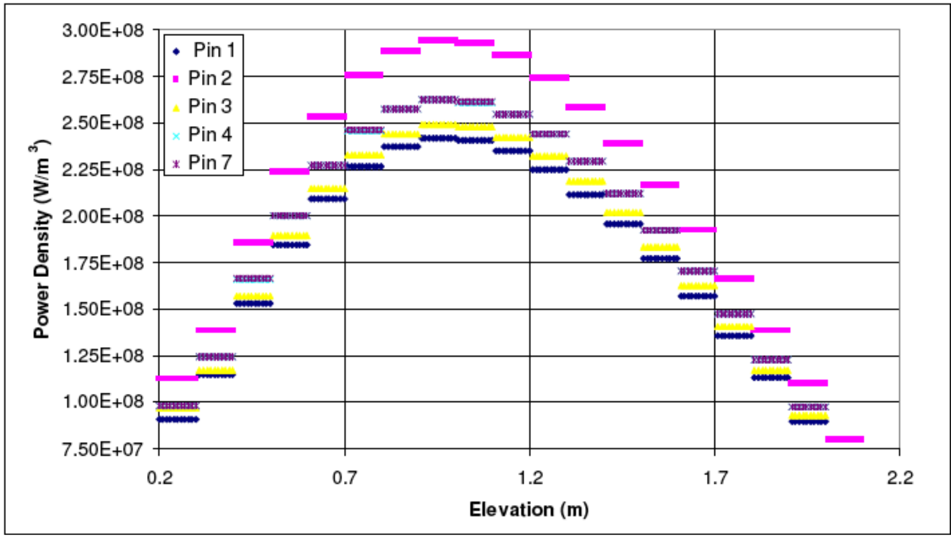


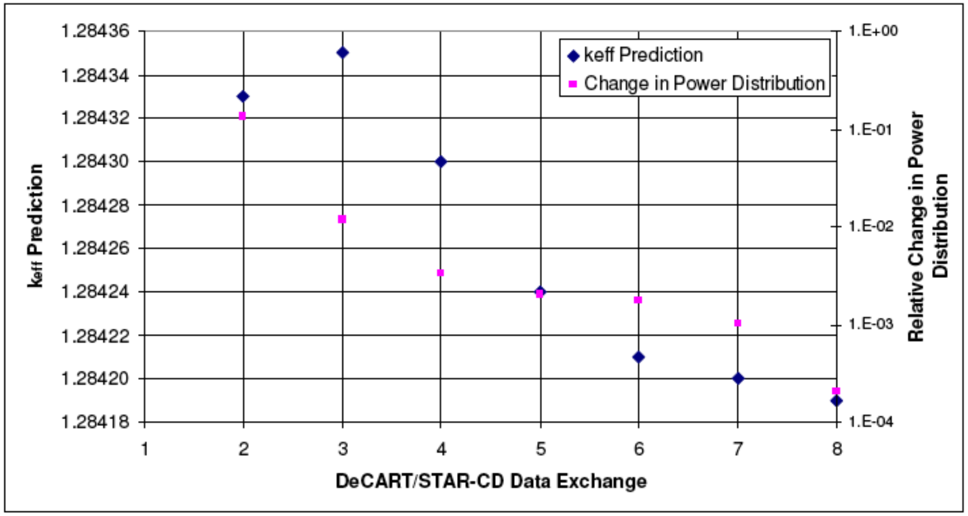


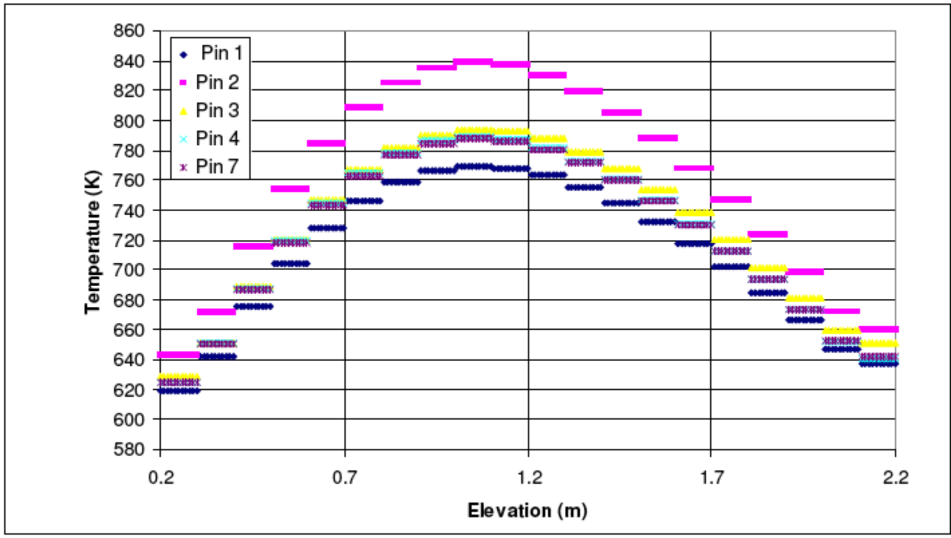


Coupled Simulation Results

- STAR-CD CFD calculation
  - 36 cores (9 quad-core nodes)
- DeCART neutronics calculation
  - 22 cores (1 core per plane)
  - Complete calculation required 2.25 hours (wall clock time)

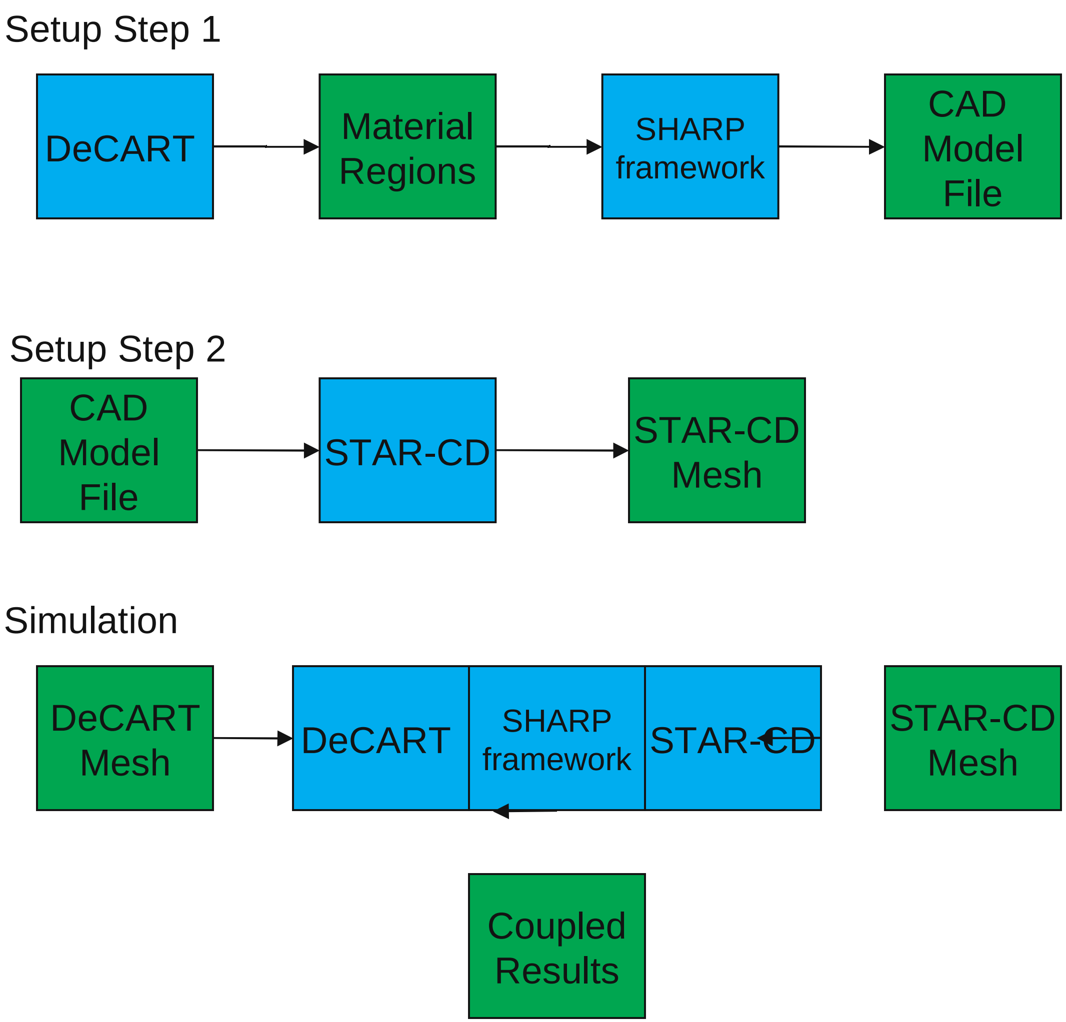






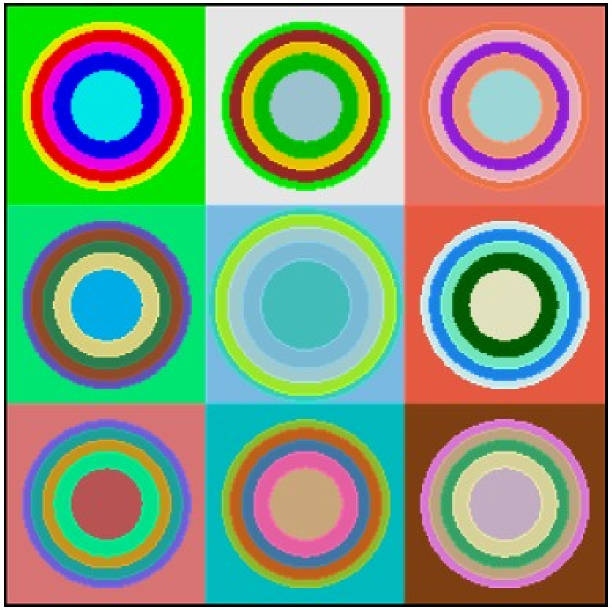
Initial Model Generation and Coupling Strategy

Allow unaligned (and unstructured, non-conformal) meshing

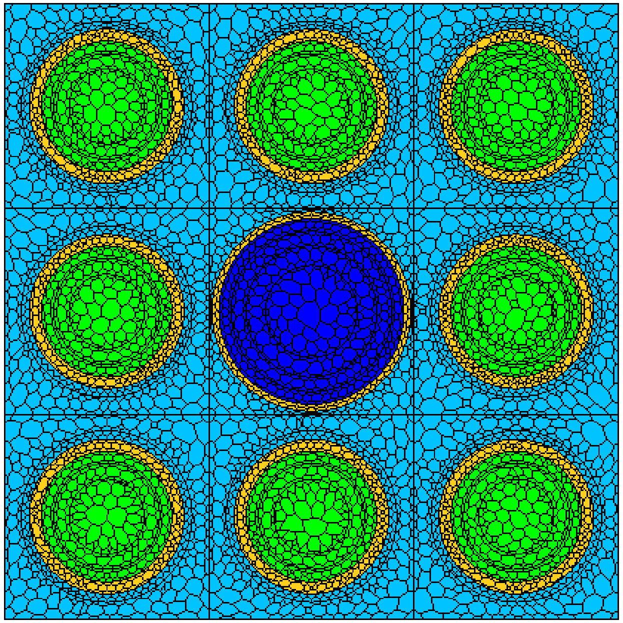


Non-conformal mesh mapping

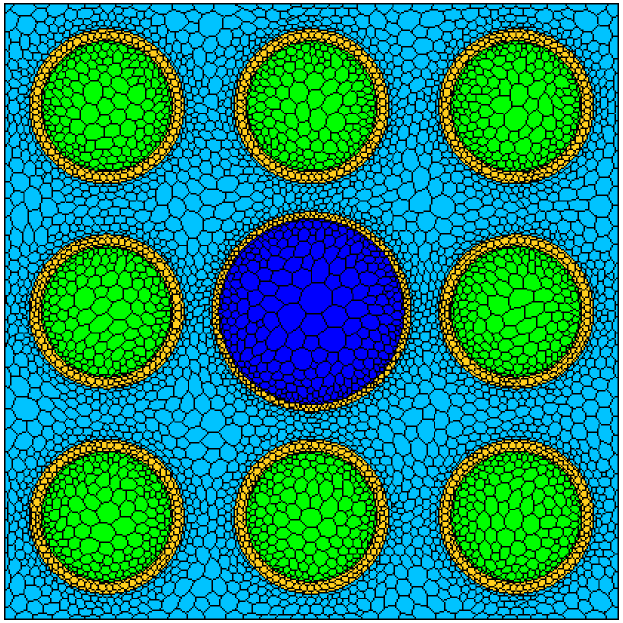
- Relax the constraint to have the DeCART and STAR-CD mesh align
- Perform inexact geometric mesh mapping
  - For the 3 x 3 LWR problem, number of mesh reduced by a factor of 4, further reduction is possible.



DeCART Spatial Mesh



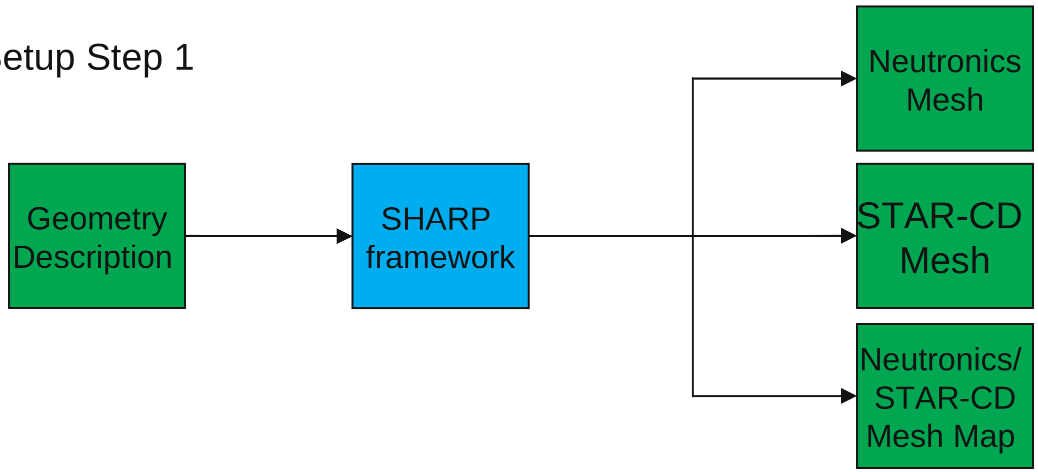
Conformal
STAR-CD Mesh



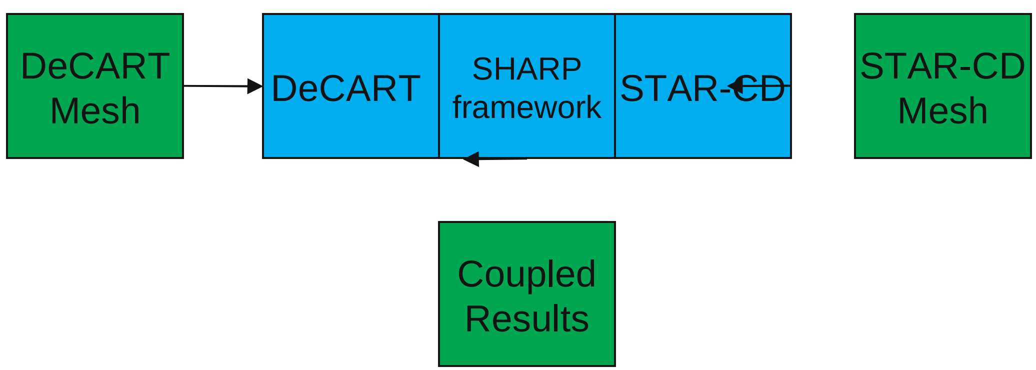
Non-Conformal
STAR-CD Mesh

Interim Strategy
Less reliance on files setup models

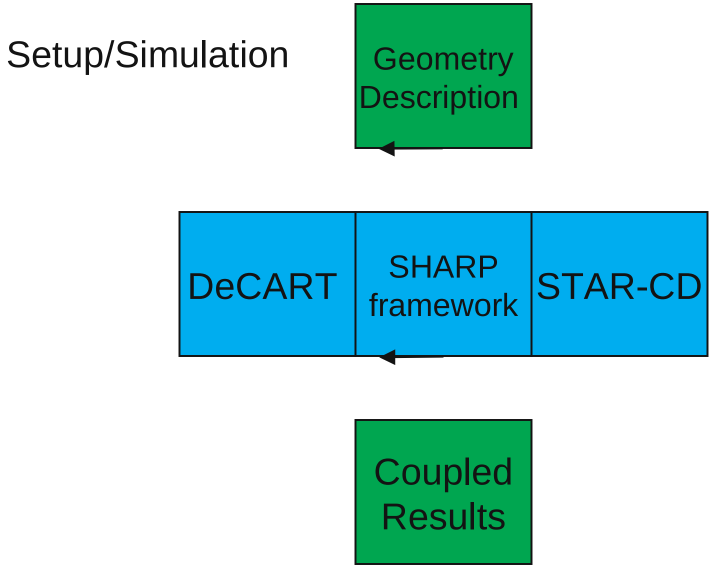
Setup Step 1



Simulation

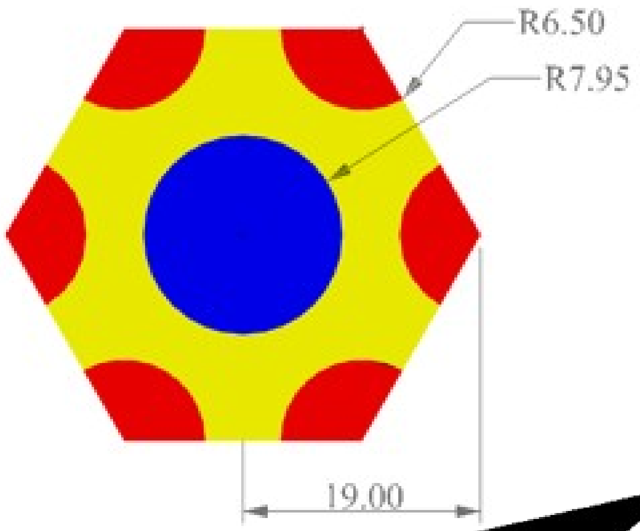


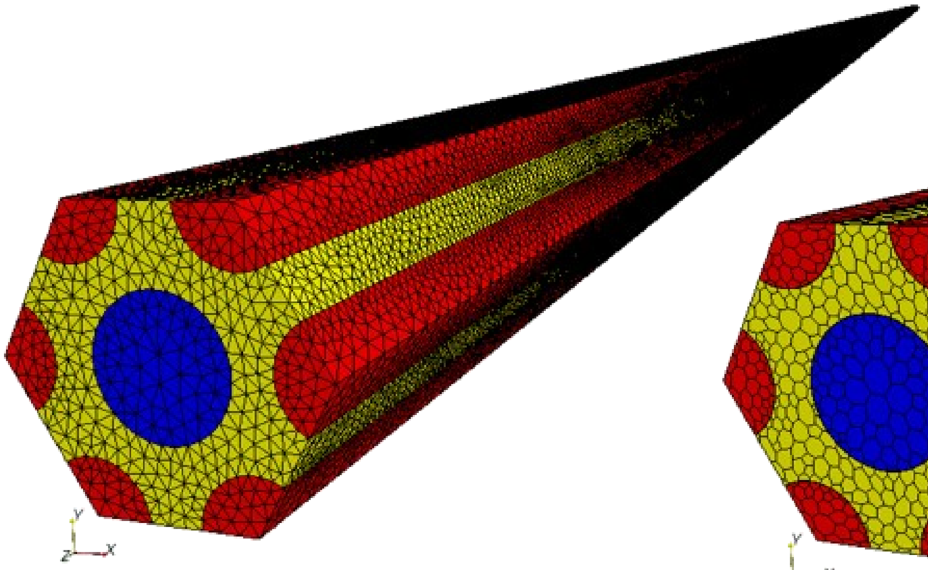
Target Coupling Strategy

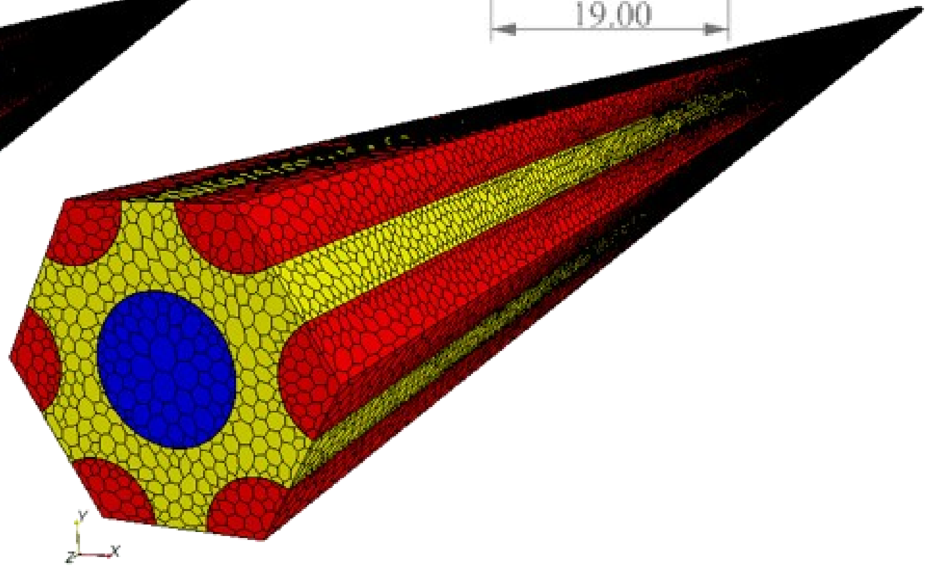


Single Channel Simulations for Selection of Modeling Parameters

- Initial CFD simulations focused on a single coolant channel and the facing segments of the surrounding fuel compacts
  - Low computational cell count ➔ fast turnaround

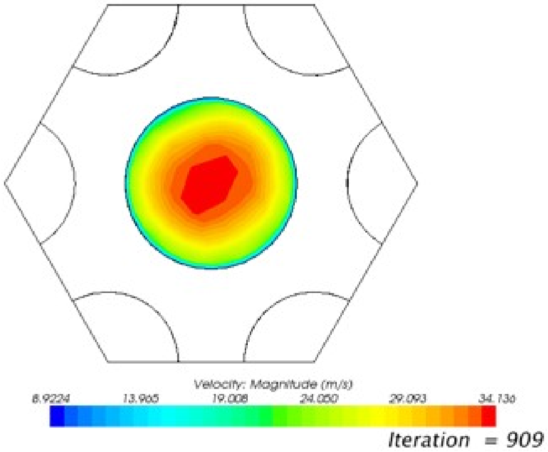


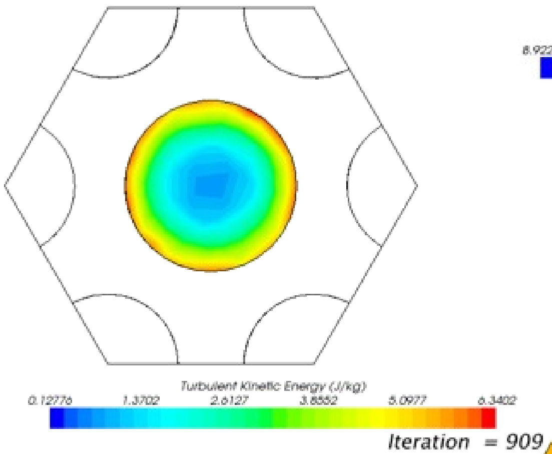


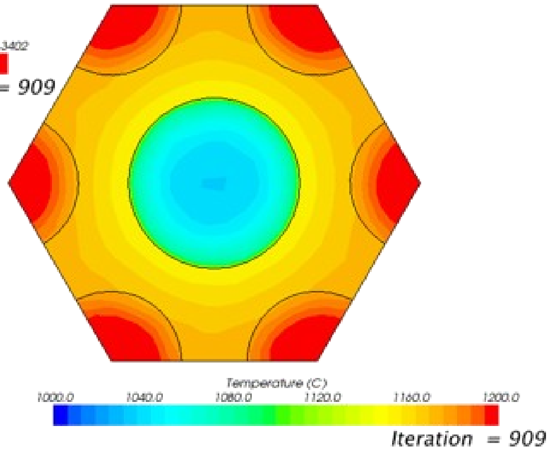


Baseline Steady State Simulations

- Segregated flow solver
- SIMPLE algorithm with Rhie-Chow interpolation for pressure-velocity coupling and algebraic multi-grid preconditioning
- 2nd-order central differencing scheme
- Realizable k-epsilon turbulence model with a two-layer all y+ wall treatment (Norris & Reynolds)
- Requires only 30 hours of total CPU time

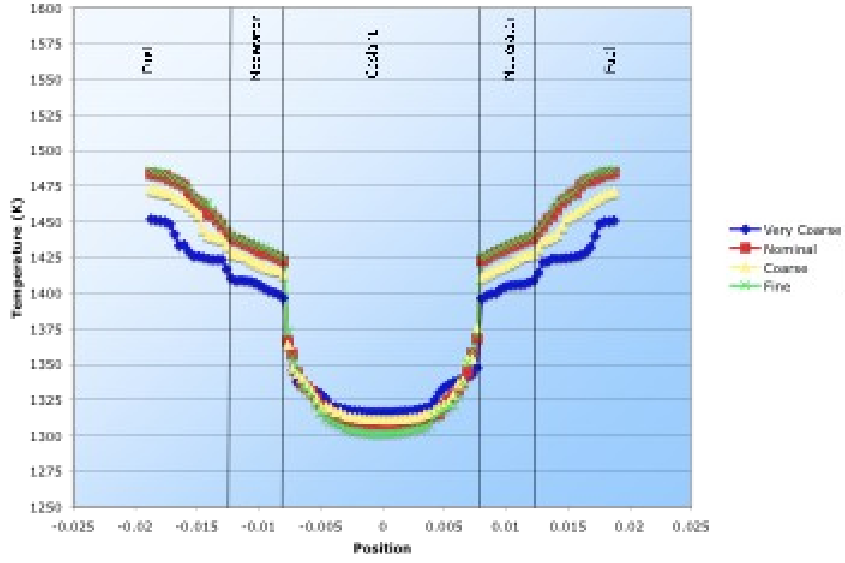


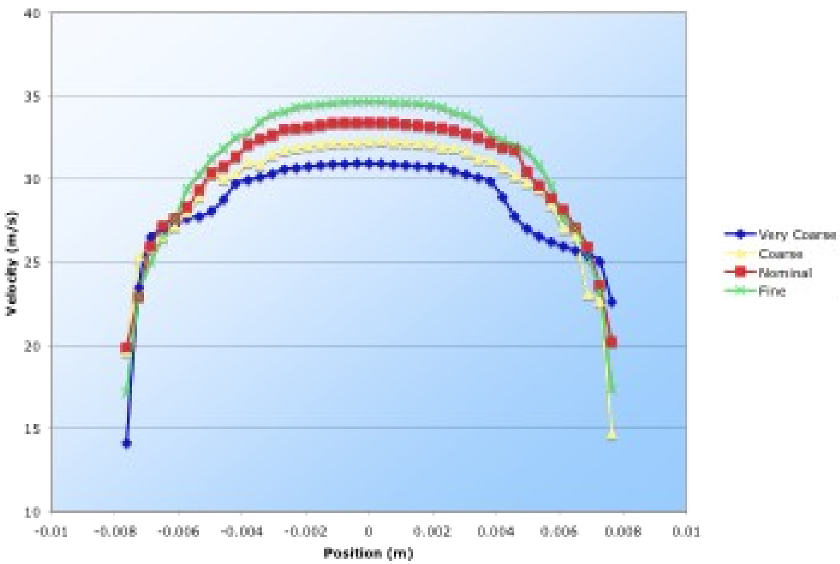


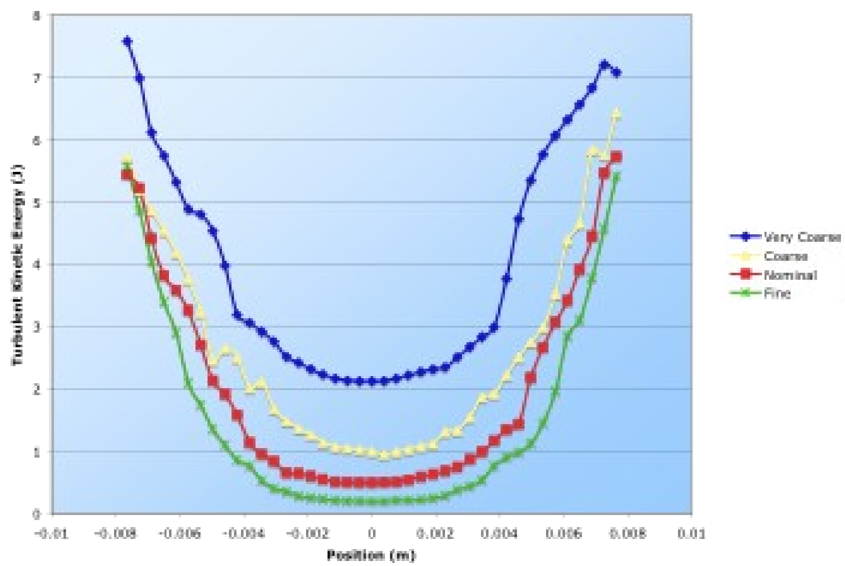


Mesh Sensitivity

Mesh	Label	Number of Coolant Cells	Number of Fuel Cells	Number of Graphite Cells
A	Very Coarse	332,602	866,088	1,215,481
B	Coarse	472,776	969,726	1,636,353
C	Nominal	718,243	1,178,336	2,378,531
D	Fine	1,218,783	1,676,533	3,876,790

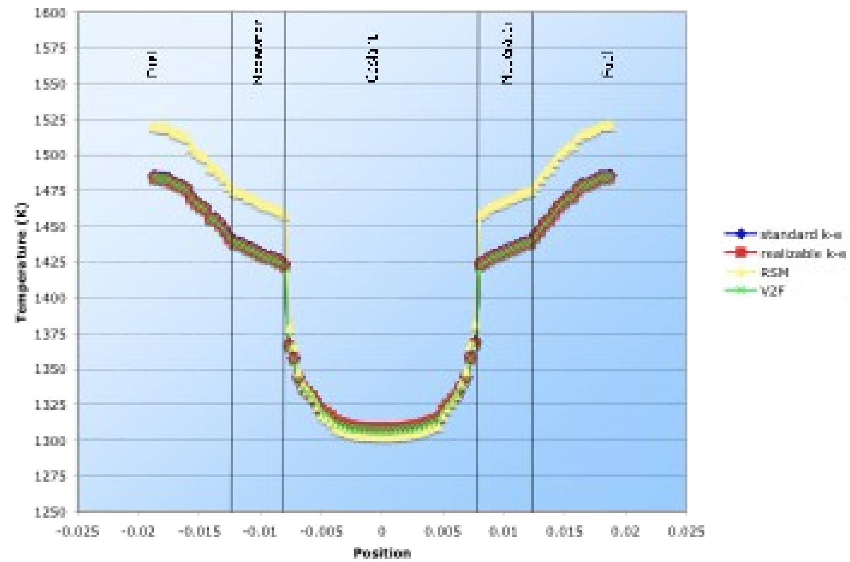


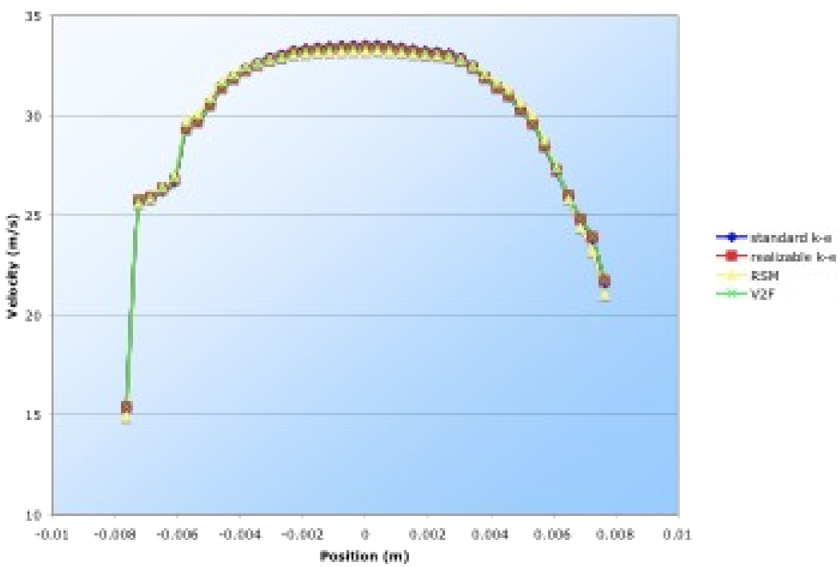


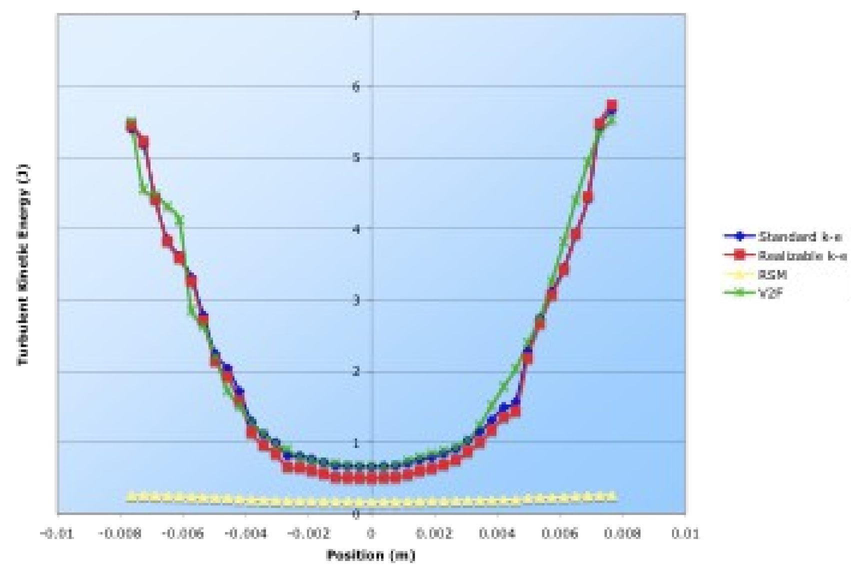


Turbulence model selection

- Consider 4 unique turbulence models
  - Two-layer realizable k-epsilon
  - Two-layer standard k-epsilon
  - Stanford V^2F
  - Algebraic Reynolds Stress Model

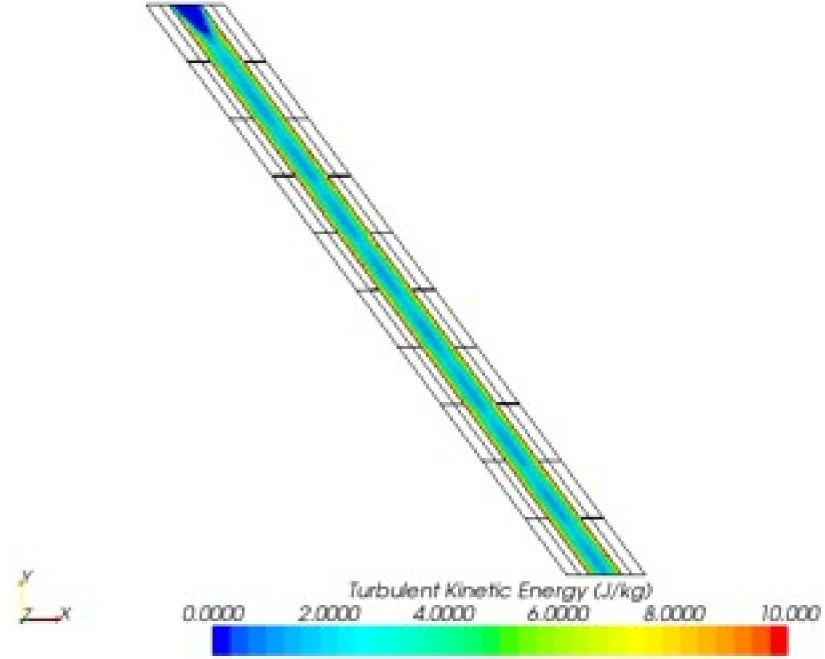


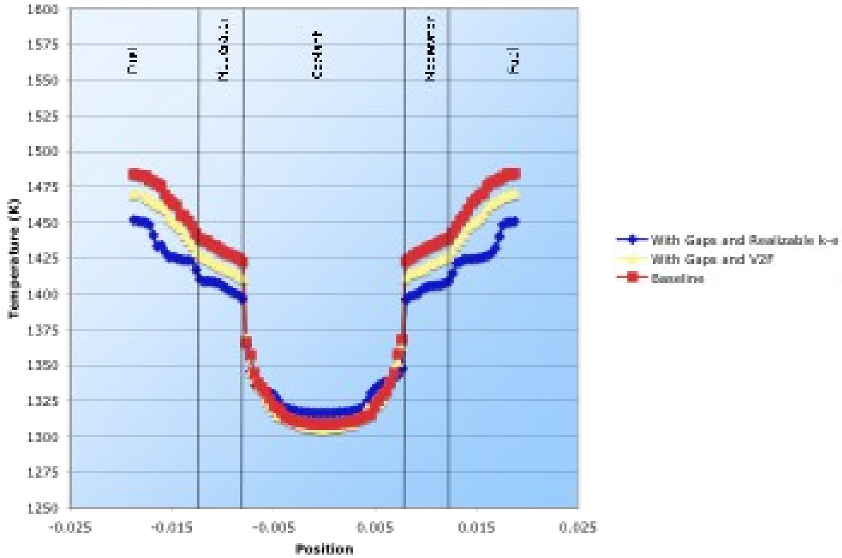


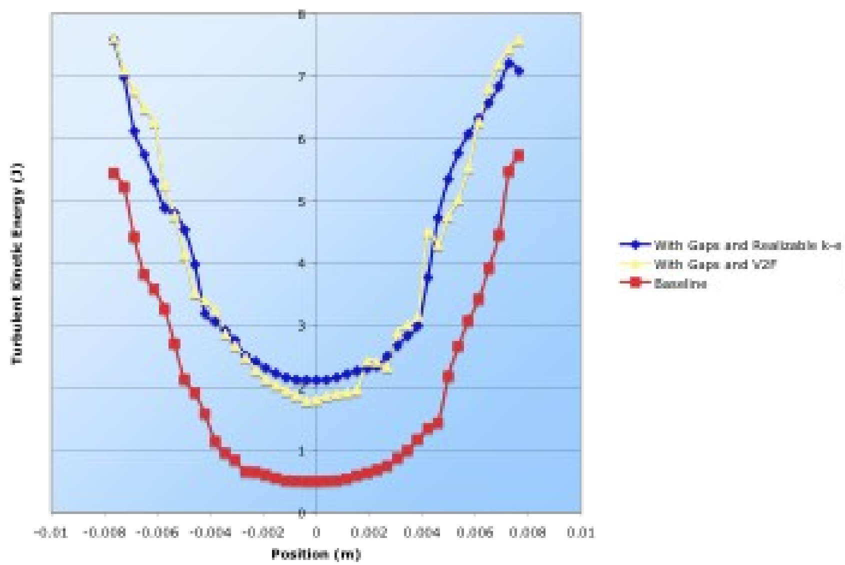


Radial gap effects

- Introduced artificially large gap between each block in the column considered in the single channel model
  - 3mm gap spacing (0.7mm maximum expected)

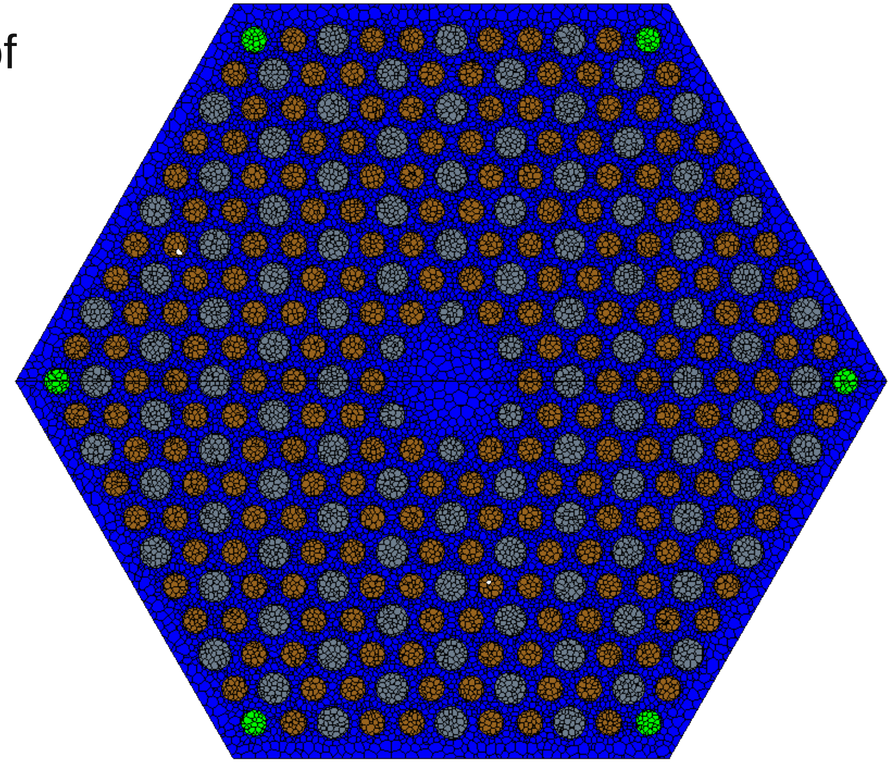


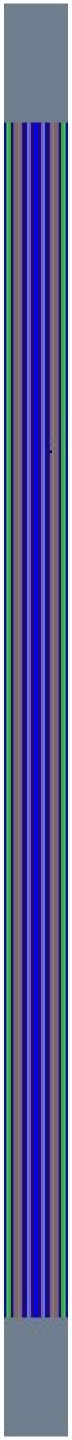




Full Block Models

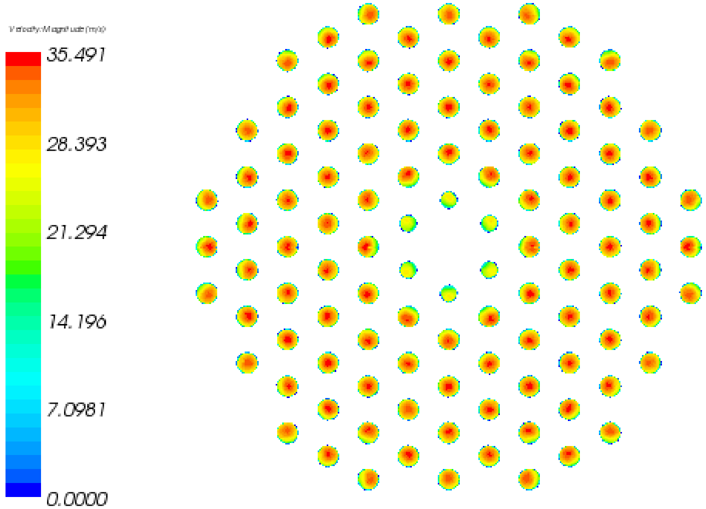
- Using meshing strategies developed for single channel, a CFD mesh describing a column of full blocks has been developed
- Uses 8.8 million computational cells
  - Polyhedral elements allow conformal meshing of solid and fluid components
    - *Improved numerical performance for conjugate heat transfer*
  - Includes upper and lower plenum volumes
  - Flow splits between channels are simulated

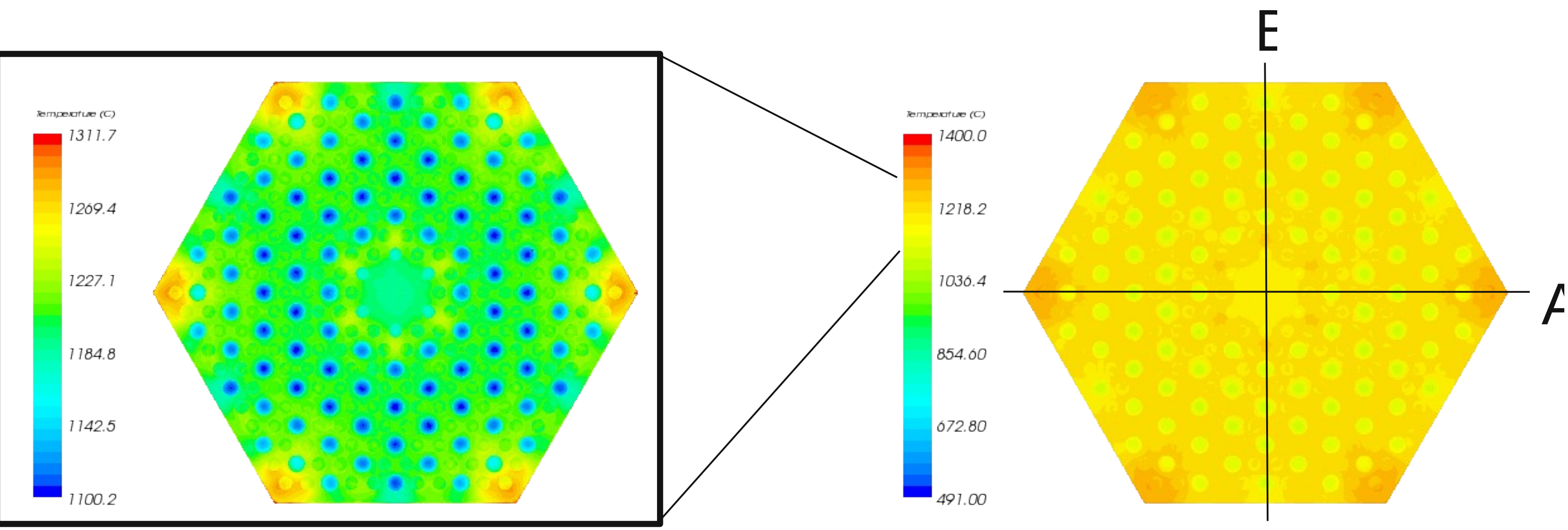


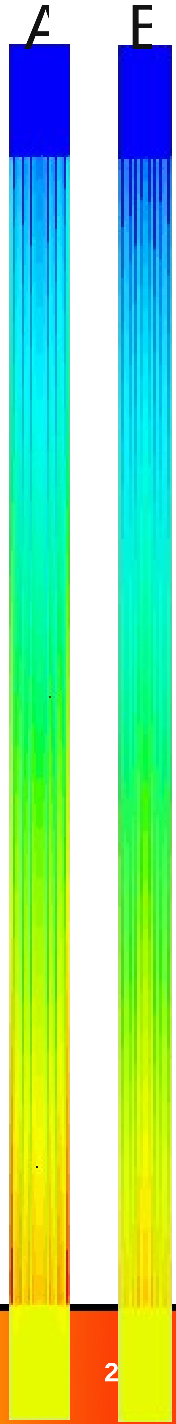


Full Block Model Results

- Assume uniform power distribution
  - Burnable poison channels treated as fuel
- Simulations require 17.5 total CPU hours on 20 cores

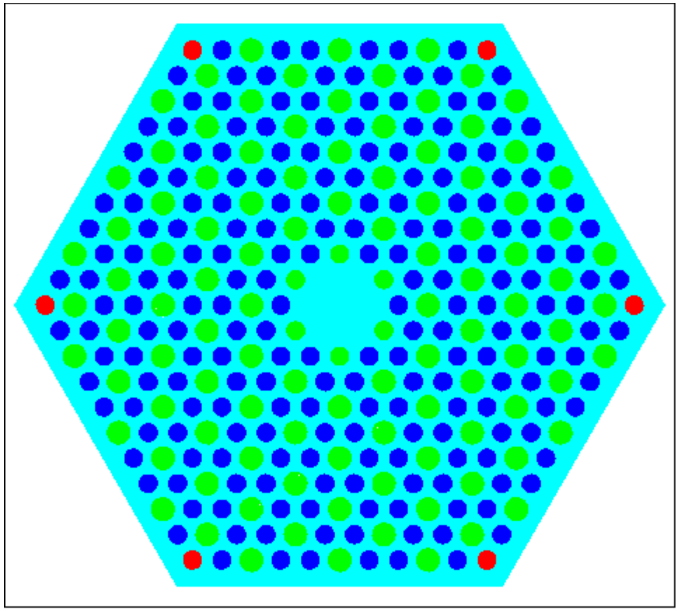


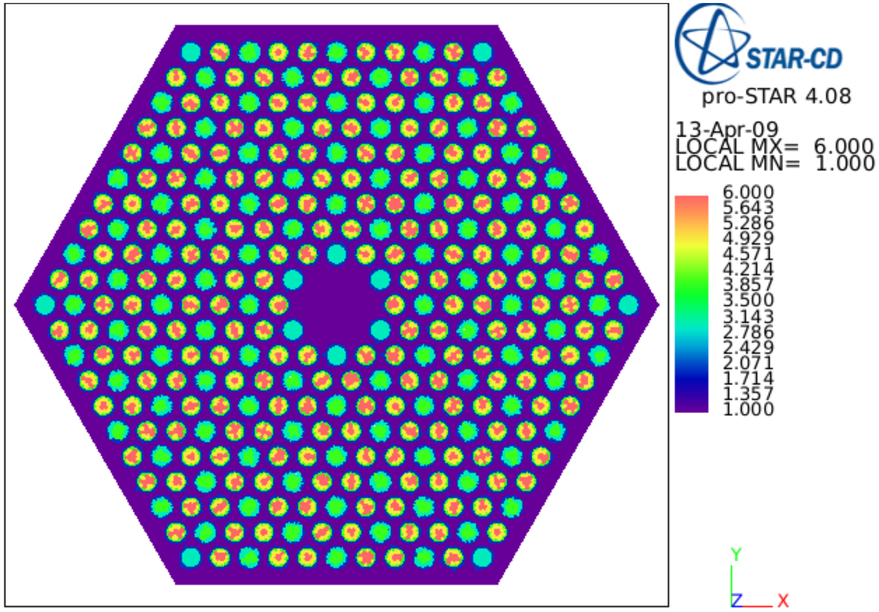




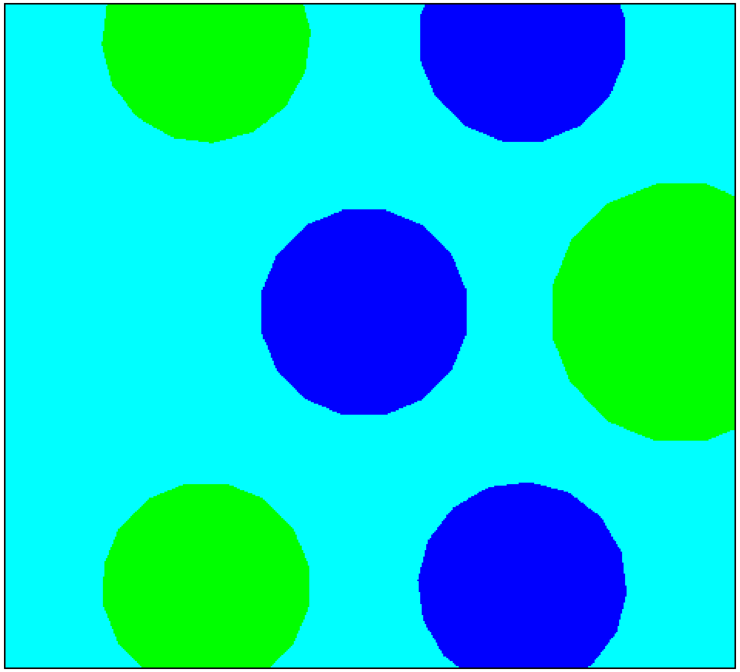
DeCART/STAR-CD Mesh Mapping

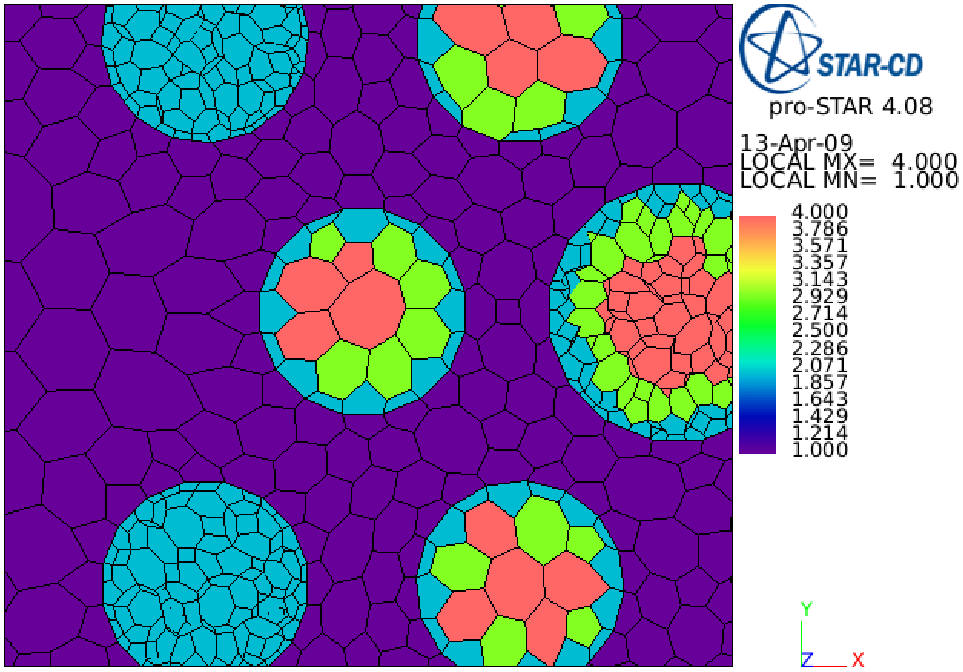
- Initial mapping utility uses a simple approach in which DeCART zones are associated with all STAR-CD cells whose centroid falls within that zones.
- Global conservation is enforced within any single material across the entire domain





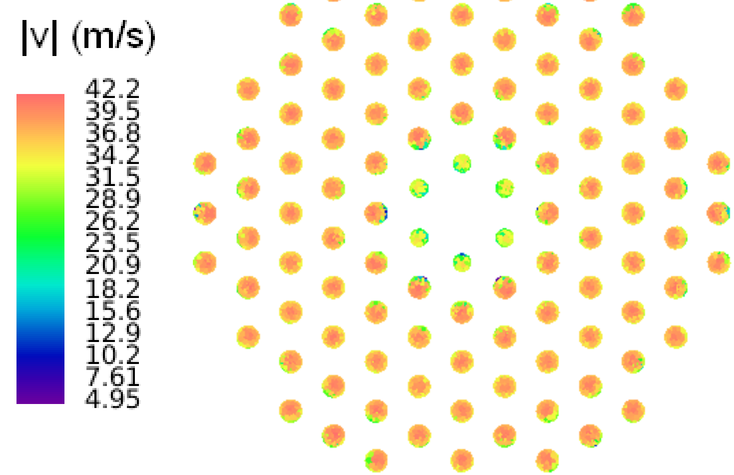
Detailed view of mapping at top of fuel block

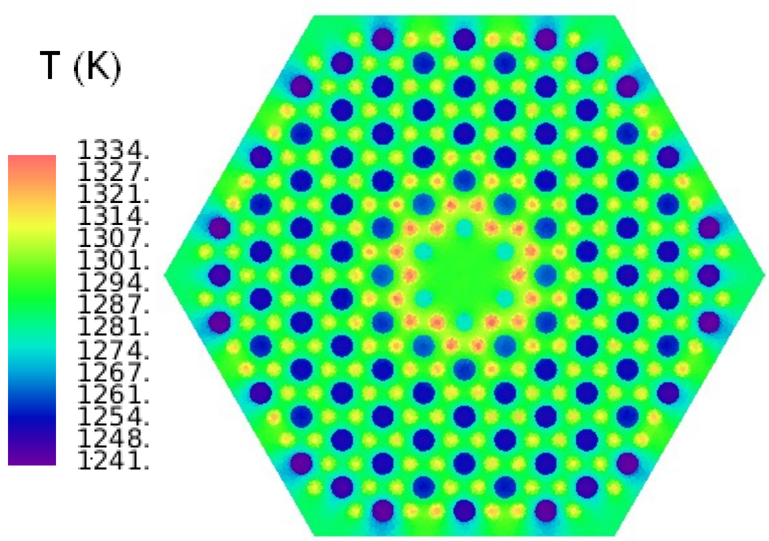


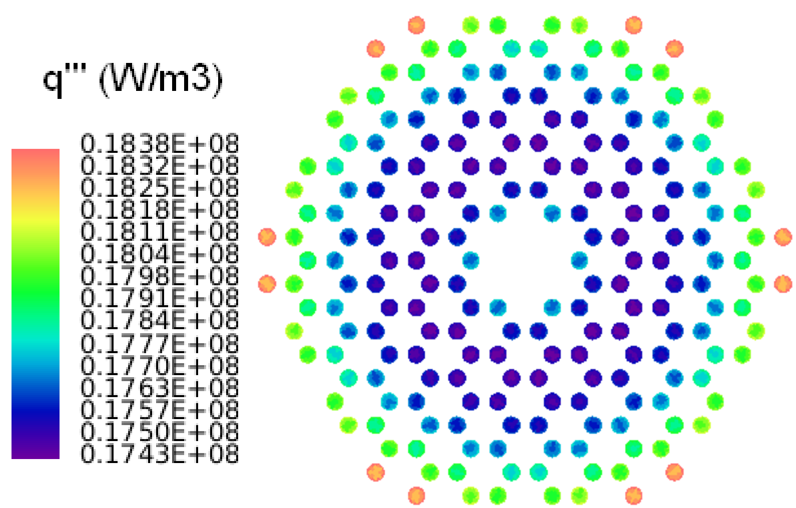


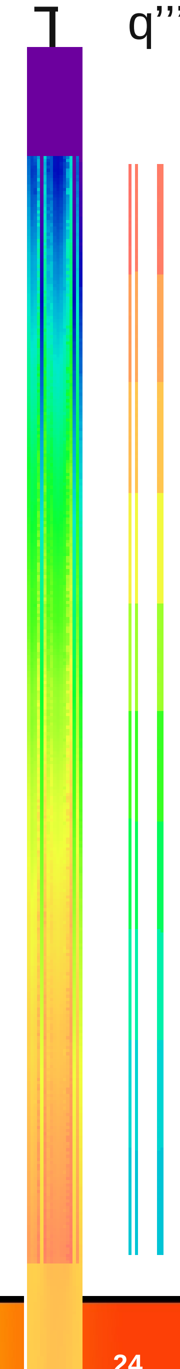
Coupled Full Block Model Results

- Power distribution from DeCART, reflects temperature feedback from CFD
- Temperature feedback exaggerated, due to greatly increased F/M ratio for single block
- After CFD initialization, coupled simulation required 4.2 hours on 32 cores for 9 data exchanges









Key Achievements and Findings in Thermofluids Modeling and Coupling

- Developed staged integration strategy for incorporation of STAR-CD/STAR-CCM+ into SHARP framework
  - *Build upon NNR experience*
  - *Focus on improvement of simulation and model development efficiency*
- Demonstrated methodology for generation of computational meshes describing prismatic VHTR geometry from CAD data for both DeCART and STAR-CD.
- Completed scoping studies of mesh resolution effects and turbulence model performance
  - *Identified baseline mesh resolution paramters*
  - *Selected realizable k-epsilon model with two-layer (Norris & Reynolds) wall treatement*
- Developed hexagonal geometry mesh mapping tools for exchange of data between DeCART and STAR-CD
- Initiated simulation of first coupled calculation.
  - *Consider one column of fuel blocks*

Future Work

- Assess the limitations of the existing 2D-1D iteration scheme of DeCART
  - Devise a more robust iterative scheme or an alternative framework for the 3D transport calculation
- Develop enhanced parallel computation schemes for 2D MOC and 3D calculations of DeCART
- Develop an optimized, VHTR-specific scheme for iteration between neutronics and thermo-fluid simulations based on observations of convergence behavior
- Extend the DeCART library to include fission products cross sections and additional data required for depletion and kinetics analyses
- Evaluate importance of radiation heat transfer between adjacent prismatic fuel blocks relative to multi-dimensional conduction in the graphite block and convective heat transfer in the bypass flow channel as predicted by CFD mode
- Develop software (e.g., java wrapper and interface) for STAR-CD to facilitate its coupling with other physics module with minimal reliance upon native features in CFD module (in particular, mesh generation)
- Enable CFD simulations of density-driven natural convection multiple block models to capture mixed and natural convection heat transfer in low flow regions of the core and improve prediction of pressure losses
- Perform additional verification and validation analyses using HTTR and possibly Fort St. Vrain benchmark data